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MASS CONSERVATION FOR INSTANTANEOUS SOURCES
IN FEM3 SIMULATIONS OF MATERIAL DISPERSION

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MASTER

ABSTRACT

FEM3 has been used extensively for simulations of material release and dispersion from instantaneous sources, and it was noted at an early date that the inventory of total material mass changed during the first few seconds before any material could have reached an exit boundary. These failures of FEM3 to conserve mass were considered to be acceptable as long as the mass changes were only a few percent. They were attributed to numerical artifacts associated with the integration over the computational mesh to determine total mass content.

More recent cases involving the instantaneous release of high-density, two-phase material were observed to have substantial losses of a large fraction of the material mass in only one or two seconds. The material phase-change model and the omission of the $\partial p / \partial t$ term from the mass conservation equation (to preclude sound waves and permit more efficient computation) were added to the list of possible causes of the non-conservation of material mass.

This report presents the results of a systematic study in which it is shown that (1) the numerical integration errors in determining material mass content are negligible; (2) the material phase-change model by itself is not a cause of material mass variation; and (3) a linear relation between fractional mass change and fractional density change at the source center for given mesh and source geometries exists over a range of values from 10^{-5} to 10^{-1} . This suggests that the omission of the $\partial p / \partial t$ term from the mass conservation equation is the cause of the observed non-conservation of mass by FEM3. It is shown that these mass variations can be minimized by minimizing the initial density gradients in the source region.

As noted in the Epilogue, revisions to FEM3 that should improve mass conservation have been proposed but not implemented and tested.

INTRODUCTION

Instantaneous sources have been used to model the material release in all of the FEM3 simulations of material dispersion that the Lawrence Livermore National Laboratory (LLNL) has made for the U.S. Army Chemical Research, Development and Engineering Center (CRDEC). We noted from the beginning of this work that material mass was not perfectly conserved in the simulations during early times before there was any transport of material through the downwind exit boundary of the computational mesh. Most of this mass variation occurred during the first few seconds of each simulation. We first attributed this mass variation to a numerical artifact associated with the steep initial material concentration gradients in the source region and the linear interpolation between the mesh nodes used to determine the material mass present. This initial mass variation was negative in all of the earlier cases except one. (We will find that this exception was significant.) These mass variations were considered acceptable and not investigated further because they were only about 5 or 10 percent.

However, initial mass losses of 20 percent and more were observed in some of the later FEM3 simulations with liquid-to-vapor phase change that were made with HCN for CRDEC and with Cl_2 for another agency. We then suspected that more than a numerical artifact was involved. Perhaps the material phase-change submodel did not conserve mass. Or perhaps an assumption made in the interest of suppressing sound waves (that $\partial p / \partial t = 0$ in the mass conservation equation [1]) was a contributing factor. (However the $\partial q / \partial t$ term is retained in the equations for conservation of species where q is the mass fraction of the material present in a given phase, vapor or liquid.) We begin the following study by considering a pair of simulations recently made for CRDEC [2]: the mass decrease during the first 2.5 s was 22 percent for one and only 1.2 percent for the other.

TWO FEM3 SIMULATIONS FOR CRDEC

CRDEC requested a series of FEM3 simulations of vapor dispersion from 40 munitions randomly distributed in a target area of 5000 m². Each munition released 2 kg of material. As we explain in Ref. 2, it was necessary to approximate these 40 sources by 13 equivalent sources containing a total of 80 kg of material and to divide the target area into two halves of 2500 m² each. In the present study, we consider the 2500 m² area with six sources containing a total of 46 kg because it includes the largest source of 18 kg.

We start with Simulations 1 and 2 that are described in Table 1. As shown in that table, these simulations differ only in the values of σ_r , σ_y , and β that are used to define trivariate Gaussian distributions of material about a point 0.5 m above the ground. Simulation 1 was made before the initial evaporative cooling submodel was available for use with the material phase-change submodel [3], and the small values of σ_r and σ_y were an expedient used at that time to give initial conditions such that some of the material was in the liquid phase. Simulation 2 was made after the initial evaporative cooling option was available. As noted in Ref. 2, more than 20 percent of the material mass was "lost" during the first 2.5 s in No. 1 but only about 1 percent in No. 2. For the present study, the six-source halves of Nos. 1 and 2 were rerun for a few seconds using the same version of FEM3 with both phase change and initial evaporative cooling. The results are shown in Fig. 1 which shows a total mass loss of about 35 percent for No. 1 and a loss of less than 1 percent for No. 2. The corresponding masses of liquid and vapor are also shown; much more liquid is present in No. 1 which has the higher material mass concentration.

Simulations 1 and 2 required a large fraction of Cray 1 capacity and each simulation of 2 s of dispersion took about 10 minutes of machine time. Therefore, we continue this study with a series of smaller simulations based on the largest (18 kg) source in Nos. 1 and 2.

Fig. 1. Variation with time of the total, liquid, and vapor material masses for Simulations 1 and 2. The source geometries are defined by $s_r = 1$ m and $s_y = 0.5$ m in No. 1 and $s_r = 2.8$ m and $s_y = 1.4$ m in No. 2. The horizontal node spacing is 2 m in both cases.

Table 1. Descriptions of 14 simulations with instantaneous sources used in the FEM3 mass conservation study. The material was HCN, the wind speed was 1 m/s at 2 m, the ambient temperature was 0°C, and the atmosphere had "F" stability (slightly stable). The instantaneous sources were defined by the material mass fraction β at the center and the Gaussian distribution parameters σ_x (in the horizontal plane) and σ_y (in the vertical direction). "EC" means that the initial temperature distribution was determined by the initial evaporative cooling and material phase change models. "PC" means phase change and "AV" means all-vapor with respect to the material models. "+35°C" means that the initial temperature at the center of the source was 35°C above ambient and σ_x and σ_y were used to define the Gaussian temperature field. The node spacing in the horizontal plane, Δx and Δz , was one of the design variables. The vertical node spacing, Δy , ranged from 0.5 m at the bottom to 1.18 m at the top.

No.	Nodes	Elements	$\Delta x - \Delta z$ (m)	σ_x (m)	σ_y (m)	Sources	β (material mass fraction in mixture)	Init. Cond.	Mat. Model
1	9741	8000	2	1.0	0.5	6	0.48 to 0.87	EC	PC
2	9741	8000	2	2.8	1.4	6	0.0445 to 0.1334	EC	PC
3	1848	1400	2	1.0	0.5	$1/2$	0.8000	EC	PC
4	1848	1400	2	2.8	1.4	$1/2$	0.1239	EC	PC
5	6765	5600	1	2.8	1.4	$1/2$	0.1239	EC	PC
6	6765	5600	1	1.0	0.5	$1/2$	0.8000	EC	PC
7	1848	1400	2	1.0	0.5	$1/2$	0.8000	from No. 3	AV
8	1848	1400	2	2.8	1.4	$1/2$	0.1239	from No. 4	AV
9	6765	5600	1	2.8	1.4	$1/2$	0.1239	from No. 5	AV
10	6765	5600	1	1.0	0.5	$1/2$	0.8000	from No. 6	AV
11	1848	1400	2	1.0	0.5	$1/2$	0.8000	+35°C	AV
12	1848	1400	2	2.8	1.4	$1/2$	0.1239	+35°C	AV
13	6765	5600	1	2.8	1.4	$1/2$	0.1239	+35°C	AV
14	6765	5600	1	1.0	0.5	$1/2$	0.8000	+35°C	AV

COMMON FEATURES OF THE ADDITIONAL SIMULATIONS

We used the same material (HCN) and meteorological conditions as we did for Simulations 1 and 2 as described in Table 1.

We retained the vertical node spacing along the y-axis of the mesh (11 nodes in 8 m) that was used for Nos. 1 and 2. The minimum node spacing (Δy) was 0.5 m next to the ground and increased by a factor of 1.1 from node to node to a maximum of 1.18 m at the top of the mesh. We assumed lateral symmetry for the 18-kg source and its dispersion field and modeled only one-half of the source and its dispersing cloud. We used a half-width of 14 m and a length of 40 m for the mesh. The center of the source was 14 m downwind of the mesh inlet. The node spacing of 2 m in the horizontal plane (Δx and Δz) that was used in Nos. 1 and 2 resulted in a computational mesh with 1848 nodes and 1400 elements for Simulations 3 and 4 as shown in Table 1. The respective values for the material mass fraction in the mixture of $\beta = 0.8$ and $\beta = 0.1239$ at the centers of the sources resulted in initial material masses of 10 kg for Nos. 3 and 4. (We chose to approximate one-half of the 18-kg sources in Simulations 1 and 2 with a mass of 10 instead of 9 kg.) Simulation 3 is similar to No. 1 with $\sigma_x = 1.0$ m and $\sigma_y = 0.5$ m while No. 4 is similar to No. 2 with $\sigma_x = 2.8$ m and $\sigma_y = 1.4$ m. (Note the inverse relation between the material mass fraction at the center (β) and the Gaussian parameters (σ_x and σ_y) for a given material mass.)

The effects of variations in horizontal node spacing were of interest so Simulations 5 and 6 with 1-m node spacing in the horizontal plane (Δx and Δz) were added. Their computational meshes had 6765 nodes and 5600 elements as noted in Table 1. The only difference in design between Nos. 3 and 6 and between Nos. 4 and 5 is the horizontal node spacing.

The Cray 1 time required for PREFEM3 and FEM3 for 2.5 s of dispersion was less than 30 s each for Nos. 3 and 4 because the pressure matrix could be solved in memory. This was not possible for Nos. 5 and 6 for which PREFEM3 plus FEM3 for 2.5 s of dispersion took about 4 min. each.

MASS CONSERVATION FOR THREE SETS OF FOUR SIMULATIONS

Phase Change with Initial Evaporative Cooling

The first set of additional simulations consists of Nos. 3 - 6 which are described above in the text and Table 1. This set was made with liquid-to-vapor phase change in combination with initial evaporative cooling [3], as was the case with Nos. 1 and 2. The variables for Nos. 3 - 6 are the node spacing in the horizontal plane (2 m for Nos. 3 and 4, 1 m for Nos. 5 and 6), the Gaussian material distribution functions ($\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m for Nos. 3 and 6, $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m for Nos. 4 and 5), and the material mass fraction specified at the source centers ($\beta = 0.8$ for Nos. 3 and 6, $\beta = 0.1239$ for Nos. 4 and 5).

We should consider the variation of initial material mass as a function of the horizontal node spacing and the Gaussian source parameters before we examine the mass variations with time for Simulations 3 - 6. The initial masses were almost exactly 10 kg for Nos. 3 - 5 but only 6.340 kg for No. 6. Note that $\sigma_r > \Delta x = \Delta z$ and $\sigma_y > \Delta y$ for Nos. 4 and 5 but not for Nos. 3 and 6. Therefore, the total material mass is relatively insensitive to the change from $\Delta x = \Delta z = 2$ m to $\Delta x = \Delta z = 1$ m for Nos. 4 and 5, respectively, but this is not the case for Nos. 3 and 6, respectively.

Now let us consider the mass variations with time for Simulations 3 - 6 that are shown in Fig. 2. The amount of liquid decreases and that of vapor increases in all cases. The variation of the total material mass is negligible with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m as shown in Fig. 2b for No. 4 and in Fig. 2c for No. 5. On the other hand, the total mass loss is considerable with $\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m as demonstrated in Fig. 2a for No. 3 and in Fig. 2d for No. 6. There is more liquid present in Nos. 3 and 6 because of their greater material mass concentrations (in excess of saturation concentration).

Fig. 2. Variation with time of the total, liquid, and vapor material masses for Simulations 3, 4, 5 and 6. These simulations are approximations for the region of the largest source in Nos. 1 and 2. The source geometries are defined by $\sigma_r = 1$ m and $\sigma_v = 0.5$ m for Nos. 3 and 6 and by $\sigma_r = 2.8$ m and $\sigma_v = 1.4$ m in Nos. 4 and 5. The horizontal node spacing is 2 m for Nos. 3 and 4 (as in Nos. 1 and 2) and 1 m for Nos. 5 and 6.

From the above, we conclude that with $\sigma_r = 2.8$ m there is little advantage in changing the horizontal node spacing from 2 m (No. 4) to 1 m (No. 5). With $\sigma_r = 1.0$ m the change from 2 m (No. 3) to 1 m (No. 6) results in a decrease in the percentage of transient total mass loss, but the mass loss in both cases is significant.

We propose the following geometric rule for the design of FEM3 simulations with instantaneous sources defined by trivariate Gaussian distributions about a point: $\sigma_r > \Delta x = \Delta z$ and $\sigma_y > \Delta y$. We will consider the effects of the mass fraction β and mixture density on mass conservation later.

All-Vapor with Initial Evaporative Cooling

The past experience with FEM3 and instantaneous sources had been that the greatest proportional losses of material mass were with simulations that involved phase change. The next set of four simulations was intended to try to determine the contribution, if any, of the phase-change submodel to transient material mass loss.

Simulations 7 - 10 were respectively identical to Nos. 3 - 6 except as follows: the initial velocity, temperature, and material mass fraction fields were the same but all the material was in the vapor phase (see Table 1). The change from a two-phase mixture to the vapor phase above resulted in less material mass present at zero time because the mixture density is a function of the material mass fraction and temperature through the equation of state, the perfect gas law. These reductions in initial material mass were only 2 percent for Nos. 8 and 9 relative to Nos. 4 and 5 (only 21 percent of the initial material mass was in the liquid phase in Nos. 4 and 5). There was 61 percent less initial material mass in No. 7 than in No. 3 (86 percent initial liquid) and 41 percent less initial mass in No. 10 than in No. 6 (79 percent initial liquid).

The variations of total (vapor) mass with time are presented in Fig. 3 for Simulations 7 - 10. There is a slight but negligible decrease in mass for Nos. 8 and 9 for which $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m. For Nos. 7 and 10 with

Fig. 3. Variation with time of the total (vapor) material masses for Simulations 7, 8, 9, and 10. The source geometries are defined by $\sigma_x = 1$ m and $\sigma_y = 0.5$ m in Nos. 7 and 10 and by $\sigma_x = 2.8$ m and $\sigma_y = 1.4$ m in Nos. 8 and 9. The horizontal node spacing is 2 m for Nos. 7 and 8 and 1 m for Nos. 9 and 10.

$\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m, there is slight initial increase in mass followed by a slight decrease. As we will see in a subsequent section, the density of the center of the sources for Nos. 7 and 10 first increased and then decreased. We then recalled the observed transient mass increase for an earlier simulation that was mentioned in the Introduction; it was for a source that was hotter than the surrounding atmosphere.

All-Vapor with Above-Ambient Initial Source Temperatures

The next set of four simulations, Nos. 11 - 14, were intended to demonstrate material mass conservation for sources with initial densities less than that of the surrounding air. In addition to the effect of the smaller molecular weight of HCN (27.03 g/mol vs. 28.96 g/mol for air), we had the effect of warm sources: their centers were 35°C above ambient and the surrounding initial temperature fields were determined by the appropriate Gaussian parameters σ_r and σ_y (see Table 1). Simulations 11 - 14 were respectively identical to Nos. 7 - 10 with the exception of the above initial temperature fields and, as a consequence, there were small differences in the initial material masses and velocity fields. There was less material initially present in Nos. 11 - 14 than in Nos. 7 - 10. The differences in the initial velocity fields were not significant.

The variation of material mass with time is shown in Fig. 4 for Nos. 11 - 14. There is an increase in mass with time in all four cases. It is slight in Nos. 12 and 13 with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m, and it is more pronounced in Nos. 11 and 14 with $\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m.

The density in the source regions of Nos. 11 - 14 increased with time as did the material mass in these sources. Conversely, the density in the source regions of Nos. 3 - 6 decreased with time while the material masses in these sources decreased. The results for Nos. 7 - 10 are mixed. This suggests that it is appropriate to examine the density and other fields in the source regions for these simulations.

Fig. 4. Variation with time of the total (vapor) material masses for Simulations 11, 12, 13, and 14. The source geometries are defined by $\sigma_r = 1$ m and $\sigma_y = 0.5$ m in Nos. 11 and 12 and by $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m in Nos. 13 and 14. The horizontal node spacing is 2 m for Nos. 11 and 12 and 1 m for Nos. 13 and 14.

DENSITIES AND TEMPERATURES IN THE SOURCES

Phase Change with Initial Evaporative Cooling

The variation of the air-HCN mixture density along a longitudinal line 0.5 m above the ground through the center of the source is shown in Fig. 5 for Simulations 3 - 6. The reference density of the air alone is 1.292 kg/m^3 . The density distributions are fair approximations to Gaussian distributions with $\sigma_x = 2.8 \text{ m}$ and $\sigma_y = 1.4 \text{ m}$ (Nos. 4 and 5) but are "spikes" with $\sigma_x = 1.0 \text{ m}$ and $\sigma_y = 0.5 \text{ m}$ (Nos. 3 and 6). Note that the peak density associated with the spikes is about four times the peak density associated with the Gaussian approximation. There was little movement of the clouds during the short dispersion simulations so the peak concentrations were always at the node that was at the initial center of the sources. As in Fig. 5, there never was any evidence in any of the simulations described herein of spatial oscillations in the one-dimensional plots of density, temperature, etc. at zero and later times.

The density variations with time at the central source node are presented in Fig. 6 for Nos. 3 - 6. Note the much greater initial densities and the greater rates of density decrease for Nos. 3 and 6 (with $\sigma_x = 1.0 \text{ m}$ and $\sigma_y = 0.5 \text{ m}$) than with Nos. 4 and 5 (with $\sigma_x = 2.8 \text{ m}$ and $\sigma_y = 1.4 \text{ m}$). This strongly suggests that the neglect of the term $\partial p / \partial t$ in the mass conservation equation in FEM3 may be the cause of much of the loss in mass with time in Nos. 3 and 6.

We emphasize that the differences between the density gradients $\partial p / \partial x$ in Fig. 5 and the density rates of change $\partial p / \partial t$ in Fig. 6 for Simulations 3 and 6 vs Simulations 4 and 5 are significantly greater than they appear to the eye. These differences are an artifact of the graphical plotting codes TESSERA (Fig. 5) and THPLOTX (Fig. 6) which automatically scale the vertical coordinate to give a square frame. There are similar differences between appearance and reality in some of the following figures. We will investigate the relation between $\partial p / \partial x$ and $\partial p / \partial t$ in a later section of this study.

Fig. 5. Longitudinal variation of the initial mixture density along a line through the source center in Simulations 3, 4, 5, and 6. The differences associated with 2-m node spacing for Nos. 3 and 4 (top) and 1-m node spacing for Nos. 5 and 6 (bottom) are apparent. So are the differences associated with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m for Nos. 3 and 6 vs. $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m for Nos. 4 and 5.

Fig. 6. Variation with time of the mixture density at the source center for Simulations 3, 4, 5, and 6. The initial rates of density decrease are much greater for Nos. 3 and 6 with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m than for Nos. 4 and 5 with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m. The horizontal node spacing is 2 m for Nos. 3 and 4 (top) and 1 m for Nos. 5 and 6 (bottom).

All-Vapor with Initial Evaporative Cooling

The initial temperature fields are respectively identical for Simulations 3 - 6 and Nos. 7 - 10. The variation of the temperature along a longitudinal line 0.5 m above the ground through the center of the source is shown in Fig. 7 for Nos. 3 - 10. These temperature profiles are a result of the initial evaporative cooling for the air-HCN mixtures in the sources for Nos. 3 - 6.

The variation of the density along the same line is presented in Fig. 8 for Nos. 7 - 10. These density plots are approximate mirror images of the temperature plots in Fig. 7. After zero time these density curves are smoothed with the side peaks decreasing and the central minimum increasing until the central part of the curve is flattened. Then the density decreases along the entirety of the curves with the ambient density as a lower limit.

The variation with time of the densities at the source centers are shown in Fig. 9 for Nos. 7 - 10. The density first increases and then decreases in all cases, but the initial density increase and the rate of density increase are greater for $\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m (Nos. 7 and 10) than with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m (Nos. 8 and 9). We noted above that there was a slight initial increase in material mass for Nos. 7 and 10.

In contrast to Figs. 5 and 6, the temperature scales in Fig. 7 are approximately equal as are the density scales in Fig. 8. However, the ranges of density values in Figs. 9a and 9d are about ten times the density ranges in Figs. 9b and 9c. Therefore, the initial rates of density increase for Simulations 7 and 10 are even greater, compared to those for Nos. 8 and 9, than they appear to the eye.

Fig. 7. Longitudinal variation of the initial mixture temperature along a line through the source center in Simulations 3 and 7, 4 and 8, 5 and 9 and 6 and 10. The horizontal node spacing is 2 m in (a) and (b) and 1 m in (c) and (d). The source geometries are defined by $\sigma_r = 1$ m in (a) and (d) and by $\sigma_r = 2.8$ m in (b) and (c).

Fig. 8. Longitudinal variation of the initial mixture density along a line through the source center in Simulations 7, 8, 9, and 10. The horizontal node spacing is 2 m for Nos. 7 and 8 (top) and 1 m for Nos. 9 and 10 (bottom). The source geometries are defined by $\sigma_r = 1$ m for Nos. 7 and 10 and by $\sigma_r = 2.8$ m for Nos. 8 and 9.

Fig. 9. Variation with time of the mixture density at the source center for Simulations 7, 8, 9, and 10. Note that, in contrast to Fig. 6, the initial density changes are positive. The initial rates of density increase are greater for Nos. 7 and 10 with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m than for Nos. 8 and 9 with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m. The horizontal node spacing is 2 m for Nos. 7 and 8 (top) and 1 m for Nos. 9 and 10 (bottom).

All-Vapor with Above-Ambient Initial Source Temperatures

With the source centers for Simulations 11 - 14 at 35°C above ambient and the HCN molecular weight of 27.03 g/mol, the mixture densities in the source regions of these simulations at zero time will be less than that of the surrounding air. This is demonstrated in Fig. 10 for Nos. 11 - 14. The plots are of the density variation along a longitudinal line 0.5 m above the ground through the source center. The minimum density in each case was always at the source center node during the 2-s dispersion simulations.

The variation with time of the densities at the source centers are shown in Fig. 11 for Nos. 11 - 14. Note that all the density changes are positive and that the greatest density changes and greatest initial rates of change are for Nos. 11 and 14 with $\sigma_x = 1.0$ m and $\sigma_y = 0.5$ m.

The ranges of density values in Figs. 10 and 11 are somewhat greater for Simulations 11 and 14 compared to Nos. 12 and 13.

Fig. 10. Longitudinal variation of the initial mixture density along a line through the source center in Simulations 11, 12, 13, and 14. The horizontal node spacing is 2 m for Nos. 11 and 12 (top) and 1 m for Nos. 13 and 14 (bottom). The source geometries are defined by $\sigma_r = 1$ m for Nos. 11 and 14 and by $\sigma_r = 2.8$ m for Nos. 12 and 13.

Fig. 11. Variation with time of the mixture density at the source center for Simulations 11, 12, 13, and 14. Note that, in contrast to Fig. 6, the density increases with time. The initial rates of increase are significantly greater for Nos. 11 and 14 with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m than for Nos. 12 and 13 with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m. The horizontal node spacing is 2 m for Nos. 11 and 12 (top) and 1 m for Nos. 13 and 14 (bottom).

RELATIONS BETWEEN MASS CHANGE AND SOURCE DENSITY CHANGE

The term $\partial\rho/\partial t$ is not included in the present FEM3 model as we have noted in the Introduction. We have seen in some figures, especially Fig. 6a for Simulation 3 and Fig. 6d for Simulation 6, that large changes in mixture density can take place in a fraction of a second. We have also seen in Figs. 2a and 2d that there were large losses of total mass for Nos. 3 and 6 during the first fraction of a second. We will investigate the relation between the observed mass changes and the simultaneous changes in source center mixture densities on a systematic basis. The node at the source center for which β is specified has most of the initial material mass associated with it in the cases of Simulations 3 - 6 and 11 - 14 as shown in Figs. 5 and 10. This is not necessarily the case for Nos. 7 - 10 as shown in Fig. 8. We will determine the relations, if any, between $(1/M)\partial M/\partial t$ and $(1/\rho)\partial\rho/\partial t$ where M is the total material mass and ρ is the mixture density at the source center.

The total material masses and the corresponding source center densities for 0 and 0.25 s are listed in Table 2 for Simulations 3 - 14. In addition, the fractional changes of total material mass and source center density are given where

$$\Delta M/M = [M(0.25s) - M(0s)]/M(0s)$$

and

$$\Delta\rho/\rho = [\rho(0.25s) - \rho(0s)]/\rho(0s) \quad .$$

The time steps for these calculations were $\Delta t = 0.025$ s with $\Delta x = \Delta z = 1$ m and $\Delta t = 0.05$ s with $\Delta x = \Delta z = 2$ m.

For the first set of four simulations with initial evaporative cooling and phase change, Nos. 3 - 6, all of the mass and density changes during the first 0.25 s are negative. The changes for $\beta = 0.1239$, $\sigma_r = 2.8$ m, and $\sigma_y = 1.4$ m (Nos. 4 and 5) are negligible (less than one percent) but those for $\beta = 0.8$, $\sigma_r = 1.0$ m, and $\sigma_y = 0.5$ m (Nos. 3 and 6) are substantial.

Table 2. Material mass and source center density changes between 0 and 0.25 s for Simulations 3 - 14 and variations "M" is the total material mass and "ρ" is the source center density. The ambient air density in all cases was 1.292 kg/m³. The design variations from the set of Nos. 3 - 14 are described in the β and Temperature columns for the initial conditions at the source center.

No.	M(kg)		$(\frac{\Delta M}{M(0s)})$	Initial source center conditions		ρ(kg/m ³)		$(\frac{\Delta \rho}{\rho(0s)})$
	0s	0.25s		β	T(°C)	0s	0.25s	
3	10.118	6.528	-0.355	0.8		5.810	3.118	-0.463
4	10.050	10.037	-0.001	0.1239		1.614	1.602	-0.007
5	10.022	10.010	-0.001	0.1239		1.614	1.601	-0.008
6	6.340	5.090	-0.197	0.8		5.810	2.619	-0.549
7	3.931	4.008	+0.020	0.8		1.294	1.364	+0.054
8	9.831	9.806	-0.003	0.1239		1.470	1.473	+0.002
9	9.803	9.778	-0.003	0.1239		1.470	1.472	+0.001
10	3.757	3.766	+0.002	0.8		1.294	1.385	+0.070
11	3.346	3.439	+0.028	0.8	35	1.083	1.137	+0.050
12	8.420	8.435	+0.002	0.1239	35	1.135	1.144	+0.008
13	8.396	8.402	+0.001	0.1239	35	1.135	1.144	+0.008
14	3.204	3.258	+0.016	0.8	35	1.083	1.159	+0.070
3A	4.970	4.107	-0.174	0.6		3.164	2.355	-0.256
3B	2.642	2.430	-0.080	0.4		2.226	1.926	-0.135
11A	3.155	3.289	+0.042	0.8	70	0.973	1.049	+0.078
11B	4.242	4.062	-0.042	0.8	-70	1.643	1.529	-0.069
11C	5.500	4.762	-0.134	0.8	-140	2.506	2.005	-0.200
6A	3.829	3.475	-0.092	0.6		3.164	2.180	-0.311
6B	2.246	2.149	-0.043	0.4		2.226	1.827	-0.179
4A	127.367	120.012	-0.058	0.9		10.743	7.953	-0.260
4B	77.986	76.453	-0.020	0.7		4.069	3.663	-0.100
4C	48.768	48.321	-0.009	0.5		2.606	2.481	-0.048
5A	124.140	118.129	-0.048	0.9		10.743	7.464	-0.305
5B	77.617	76.126	-0.019	0.7		4.069	3.613	-0.112
5C	48.622	48.170	-0.009	0.5		2.606	2.466	-0.054

The next set of four simulations, Nos. 7 - 10, are with the initial temperature fields respectively identical to those for Nos. 3 - 6 but all the material is in the vapor phase. The results are mixed. The mass changes for $\beta = 0.1239$, $\sigma_r = 1.0$ m, and $\sigma_y = 0.5$ m (Nos. 7 and 10) are positive but those for $\beta = 0.8$, $\sigma_r = 2.8$ m, and $\sigma_y = 1.4$ m (Nos. 8 and 9) are negative. All of the density changes at the source centers are positive. In view of these mixed results and the complexity of the temperature and density fields noted in the preceding section, we will not consider Nos. 7 - 10 further.

The third set of four simulations, Nos. 11 - 14, are all-vapor simulations with initial source densities less than that of the ambient air, principally because of the above-ambient source center temperatures. All of the mass and source center density changes are positive. The changes for $\beta = 0.1239$, $\sigma_r = 2.8$ m, and $\sigma_y = 1.4$ m (Nos. 12 and 13) are negligible but those for $\beta = 0.8$, $\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m are not (greater than one percent).

The greatest changes of mass and density during the first 0.25 s were for $\beta = 0.8$, $\sigma_r = 1.0$ m, and $\sigma_y = 0.5$ m in combination with $\Delta x = \Delta z = 2$ m (Nos. 3 and 11). The variations of Nos. 3 and 11 that are listed in Table 2 (note the values of β and temperature) were added as a set of five additional simulations to define the curve between Nos. 3 and 11A in Fig. 12. The result is a smooth curve that goes through the point $\Delta M/M = 0 = \Delta \rho/\rho$. This curve is approximately linear for $-0.05 < \Delta M/M < +0.05$ and $-0.1 < \Delta \rho/\rho < +0.1$ and is nonlinear for the larger negative values of $\Delta M/M$ and $\Delta \rho/\rho$. Note that the point for No. 11C (a very cold and quite dense initial source center with all material in the vapor phase) lies between the points for Nos. 3A and 3B (phase change with initial evaporative cooling). Therefore, the phase-change submodel by itself is not responsible for the non-conservation of mass by FEM3.

The changes of mass and density during the first 0.25 s were also appreciable for $\beta = 0.8$, $\sigma_r = 1.0$ m, and $\sigma_y = 0.5$ m with $\Delta x = \Delta z = 1$ m (Nos. 6 and 14). Two variations of No. 6 with different β values were added to the

Fig. 12. Fractional changes in mass vs. fractional changes in source center density during the first 0.25 s. The solid curves are for $\sigma_r = 1$ m and $\sigma_y = 0.5$ m. The dashed curves are for $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m, and are presented in detail in Fig. 13. Simulations 3 and its variations and 6 and its variations are with phase-change. Simulations 11 and its variations and 14 are with the all-vapor material submodel.

Fig. 13. Fractional changes in mass vs. source center density during the first 0.25 s for simulations with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m. Simulations 4, 5, and their variations are with phase change. Simulations 12 and 13 are with the all-vapor material submodel.

list of simulations as shown in Table 2. The results for No. 6, its variations 6A and 6B, and No. 14 are also plotted in Fig. 12. Comparison of the curve 6 - 14 with curve 3 - 11A shows that changing from $\Delta x = \Delta z = 2$ m to $\Delta x = \Delta z = 1$ m results in approximately doubling the fractional density change required to give a specified fractional change in mass. Note that Nos. 3, 3A, 3B, 6, 6A, and 6B are with initial evaporative cooling and phase change. Also note that $\beta = 0.8$ for Nos. 3 and 6, $\beta = 0.6$ for Nos. 3A and 6A, and $\beta = 0.4$ for Nos. 3B and 6B.

The fractional changes in mass and density for all the simulations with $\beta = 0.1239$, $\sigma_r = 2.8$ m, and $\sigma_y = 1.4$ m (Nos. 4, 5, 8, 9, 12, and 13) were negligible (less than one percent). We decided to extend the curve between Nos. 4 and 12 by means of large increases in the total material mass and source center density. We did this by means of the three variations of No. 4 (different β values) listed next to the bottom of Table 2. The result is the curve 4A - 12 shown in Fig. 13. This demonstrates that, even with a good match between the Gaussian source parameters (σ_r and σ_y) and the mesh node spacing (Δx , Δy , Δz), it is possible to have transient losses of several percent of material mass if the mixture density at the center of a source is several times the ambient air density. Such high density mixtures are characteristic of spills of cryogenic liquids or liquids with low boiling points that flash vaporize and form a two-phase mixture with a large liquid fraction.

Simulation 5 is identical to No. 4 and Simulation 13 is the same as No. 12 except that the horizontal mesh spacing (Δx and Δz) is decreased from 2 to 1 m. The three variations of No. 5 listed at the bottom of Table 2 (different β values) were added as counterparts of the variations of No. 4. The results of $\Delta M/M$ vs. $\Delta p/p$ for Simulation 5, its three variations, and No. 13 are presented together with those for Nos. 4, its three variations, and No. 12 in Fig. 13. With $\sigma_r = 2.8$ and $\sigma_y = 1.4$ m, the change in horizontal mesh spacing from 2 m (curve 4A - 12) to 1 m (curve 5A - 13) did not result in as great a proportional decrease in mass loss as with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m (compare Figs. 12 and 13).

SOURCES WITH NEUTRAL AND ALMOST-NEUTRAL BUOYANCY

The curves in Figs. 12 and 13 relating fractional changes in material mass and source center density pass through the point 0,0. We will study five additional simulations with values of $\Delta M/M$ and $\Delta \rho/\rho$ that are in the vicinity of this point. We will use the same geometry as Simulations 3, 11, and their variations: a mesh with 1848 nodes, 1400 elements and $\Delta x = \Delta z = 2$ m together with the Gaussian source parameters $\sigma_x = 1$ m and $\sigma_y = 0.5$ m. These simulations had the greatest fractional changes of material mass, as shown in Fig. 12.

We will consider one simulation in which the source has neutral buoyancy and others with sources that have slightly positive or slightly negative buoyancies. We will use the all-vapor material submodel in an isothermal dispersion process. Under these conditions the buoyancy is governed by the vapor molecular weight and the material concentration. The molecular weight of air has a value of 28.96 g/mol in the version of FEM3 that we are using (not 28.95 g/mol as stated in Ref. 4). We chose a vapor molecular weight of 28.95 g/mol for Simulation 15, 28.96 g/mol for No. 16, and 28.97 g/mol for No. 17. We later added No. 15A with $M_v = 28.959$ g/mol and No. 17A with $M_v = 28.961$ g/mol. These molecular weights differ from that of air by ± 0.01 g/mol for Nos. 15 and 17 and by ± 0.001 g/mol for Nos. 15A and 17A. We used $\beta = 0.8$ for the mass concentration of the material in all cases. This resulted in perturbations from neutral buoyancy at the source center of less than 3 parts in 10^4 for No. 15 (positive) and No. 17 (negative). Similarly, the perturbations from neutral buoyancy were less than 3 parts in 10^5 for Nos. 15A and 17A.

The variation of material concentration at the source center is shown in Fig. 14a for Simulations 15 - 17 including Nos. 15A and 17A (the five curves are identical with respect to the precision possible in the figure). Note that the variations of source center density shown in Fig. 14b-c for Nos. 15A and 15 (above) are "mirror images" of those in Figs. 14e-f for Nos. 17A and 17

Fig. 14. Variation with time of material concentration and mixture density at the source centers for five simulations (Nos. 15, 15A, 16, 17, and 17A) with neutral or almost-neutral buoyancy. (a) Variation of concentration for all five simulations, (b) - (f) Mixture density variations for Nos. 15A, 15, and 16, 17A, and 17.

(below). Furthermore, these four curves appear to have the same shape, but this appearance is deceptive because the ranges of densities for Nos. 15 and 17 are ten times those of Nos. 15A and 17A. Also note the slight linear increase of density with time in Fig. 14d for No. 16 with neutral stability. This slow and small increase in density is explained below.

Fig. 15 shows the longitudinal variation along a line through the source center of the longitudinal velocity component at 2 s for Simulations 15 - 17 and variations. The velocity was equal to zero between -20 and -16 m at zero time; this constraint was released at the beginning of the dispersion simulations. Note the similarity of the curve for velocity in Fig. 15a and the curve for density at zero time for the neutral buoyancy simulation, No. 16, in Fig. 15d. The density in this simulation varied slightly in space and with time as determined by the slightly nonsteady coupled velocity and pressure fields. The longitudinal variations of density at zero time for Nos. 15A, 15, 17A, and 17 are shown in Figs. 15b-c and 15e-f, respectively. As in Fig. 14, these plots for Nos. 15 and 17 and their variations are mirror images of each other, and the ranges of density values for Nos. 15 and 17 are ten times those for Nos. 15A and 17A. Therefore, the density gradients in the sources of Nos. 15 and 17 are ten times those of Nos. 15A and 17A. The longitudinal variations of density upwind and downwind of the sources in Figs. 15b-c and 15e-f are comparable to that in Fig. 15c, but are not as noticeable because of the different scales.

The variation with time of material mass and source center density for Simulations 15, 16, and 17 are plotted in Fig. 16. We saw in Fig. 14(a) that the variation with time of the material concentration at the source center was essentially identical all three simulations. We see here that the mass and density are constant at this scale for the neutrally-buoyant case, No. 16. With equal molecular weights for air and vapor, material diffusion does not change mixture density but it does change material mass distribution. There is no change of mass at this scale; therefore, the effect of any numerical artifact should be evident at only an expanded scale. On the other hand the

Fig. 15. Longitudinal variation of wind speed and mixture density through the center of the source (at $x = -18$ m). (a) Wind speed at 2 s for all five simulations. (b) - (f) Mixture density at 0 s for No. 15A, 15, 16, 17A, and 17.

Fig. 16. Variation with time of material mass (solid lines) and mixture density (dashed lines) at the source center for Simulation 15 ($M_V = 28.95$ g/mol), 16 ($M_V = 28.96$ g/mol), and 17 ($M_V = 28.97$ g/mol).

mass and density variations for Nos. 15 and 17 are mirror images of each other. Therefore, material mass conservation in FEM3 is probably affected by the omission of the $\partial\rho/\partial t$ term for the mass conservation equation, even with these small variations in density.

We therefore extended the analysis in Table 2 and Figs. 12 and 13 as shown in Table 3 and Fig. 17. The data for Simulations 15 - 17 and their variations together with Simulations 3, 11 and their variations are presented in Table 3. There is a need for greater precision in Table 3 because of the small values of $\Delta M/M$ and $\Delta\rho/\rho$ for Nos. 15 - 17 and their variations. The absolute values of the fractional variations of material mass and source center density from Table 3 (with the exception of those for No. 16) are plotted on log-log scales in Fig. 17. It is shown that $\Delta M/M$ is, to a very good approximation, linearly related to $\Delta\rho/\rho$ over 6 orders of magnitude. The points on and near the straight line with a slope of unity represent simulations with both positive and negative source buoyancy and with and without phase change.

It is also shown in Table 3 that any numerical artifacts, to which the nonconservation of material mass in FEM3 was initially attributed, are not evident at the $\Delta M/M$ and $\Delta\rho/\rho$ values for Nos. 15 and 17 on the order of 10^{-5} . On the other hand, some numerical noise is evident in Nos. 15A and 17A for values on the order of 10^{-4} . The point for the neutral simulation, No. 16, is not plotted in Fig. 17 but it is evident from Table 3 that the linear relation plotted in Fig. 17 does not apply to this case.

We therefore conclude that we were in error when we attributed the observed nonconservation of material mass to numerical artifacts. The material mass variations in all the above simulations except that in No. 16 are probably consequences of the omission of the term $\partial\rho/\partial t$ in the FEM3 mass conservation equation. We say "probably" because we have not repeated any simulation with $\partial\rho/\partial t$ in the FEM3 mass conservation equation. Numerical artifacts are noticeable only for mixture density perturbations of 10^{-5} and smaller.

Fig. 17. The absolute values of $\Delta M/M$ and $\Delta \rho/\rho$ from Table 3, not including those of Simulation 16. The straight line through the points has a slope of unity and was drawn through the almost-coincident points for Simulations 15 and 17.

Table 3. Material mass and source center density changes between 0 and 0.25 s for ten simulations with horizontal node spacing of 2 m and Gaussian source parameters of $\sigma_r = 1$ m and $\sigma_y = 0.5$ m. The mass and density values are given to higher precision than in Table 2. Note that values for No. 16 are given twice to different degrees of precision.

No.	M(kg)		$\left(\frac{\Delta M}{M(0s)}\right)$	$\rho(\text{kg/m}^3)$		$\left(\frac{\Delta \rho}{\rho(0s)}\right)$
	0s	0.25s		0s	0.25s	
3	10.11750	6.52751	-3.548×10^{-1}	5.81006	3.11771	-4.634×10^{-1}
3A	4.96962	4.10663	-1.737×10^{-1}	3.16397	2.35524	-2.556×10^{-1}
3B	2.64171	2.43027	-8.004×10^{-2}	2.22595	1.92700	-1.348×10^{-1}
11	3.34593	3.43896	$+2.780 \times 10^{-2}$	1.08322	1.13691	$+4.957 \times 10^{-2}$
11A	3.15522	3.28927	$+4.249 \times 10^{-2}$	0.97275	1.04865	$+7.803 \times 10^{-2}$
11B	4.24193	4.06150	-4.253×10^{-2}	1.64299	1.52887	-6.946×10^{-2}
11C	5.50037	4.76247	-1.342×10^{-1}	2.50648	2.00496	-2.001×10^{-1}
15	3.69164	3.69182	$+4.876 \times 10^{-5}$	1.29145	1.29155	$+7.743 \times 10^{-5}$
16	3.69222	3.69222	0	1.29181	1.29181	0
17	3.69281	3.69263	-4.874×10^{-5}	1.29216	1.29206	-7.739×10^{-5}
15A	3.692166	3.692184	$+4.875 \times 10^{-6}$	1.291770	1.291780	$+7.741 \times 10^{-6}$
17A	3.692282	3.692265	-4.604×10^{-6}	1.291840	1.291830	-7.741×10^{-6}
16	3.692224	3.692225	$+2.708 \times 10^{-7}$	1.2918050	1.2918051	$+7.741 \times 10^{-8}$

CAUSES OF SOURCE CENTER DENSITY VARIATION

Now that we have demonstrated the correlation between fractional changes in material mass and source center density (see Figs. 12, 13, 16, and 17), let us consider possible causes of the latter.

The source center densities in this study are functions of the material concentration, material phases present, mixture temperature, material molecular weight, and pressure. The molecular weights used in this study were constants and the very small perturbations in the pressure field calculated by FEM3 had no significant effect on density. Therefore, the density variations observed were functions of changes in material concentration, material phase content, and mixture temperature. The density, concentration, phases, and temperature were determined by the combination of the mixture equation of state and the material phase change submodel. The numerical values of these variables were obtained in FEM3 from the time-dependent solutions of the conservation equations for mass, momentum, thermal energy, and species (all-vapor or liquid and vapor).

The initial momentum of the instantaneous sources in all our simulations was zero as a consequence of the initial conditions imposed. The velocity (and therefore the momentum) at the source center was negligible at 0.25 s in all cases. In contrast, there were always significant changes during the first 0.25 s of concentration, temperature, phase content, and density at the source center. This suggests that we should not look to the momentum conservation equation but to the other conservation equations for the cause of the density variations. Furthermore, we can probably neglect the advection terms in these equations.

We have noted that the $\partial p / \partial t$ term is not included in the mass conservation equation in FEM3. Therefore, the time-dependent variation of mixture density is a result of the time-dependent variations of mixture temperature and composition that are determined from the other conservation

equations (including those for the mass fraction of the species in which the $\partial q/\partial t$ term is retained). If, as suggested above, we neglect the advection terms in these conservation equations, we find that mixture temperature and content are determined by the terms for turbulent diffusion, mixing, and phase change. The diffusion and mixing terms include the gradients of temperature and species concentration. Therefore, we will investigate the possible relation between the initial density gradient next to the source center and the initial rate of density change at the center.

We will determine the initial density gradient $\Delta\rho/\Delta x$ from the zero-time values of the density at the source center node and the adjacent upwind node (see Figs. 5 and 10 for example). We will normalize this gradient by the initial source center density as follows:

$$(1/\rho)\Delta\rho/\Delta x$$

where the quantity Δx is either 1 or 2 m. The values of the normalized initial density gradients are given in Table 4. We will convert the fractional source center density change $\Delta\rho/\rho$ in Table 2 to

$$(1/\rho)\Delta\rho/\Delta t$$

where $\Delta t = 0.25$ s. The resultant values of this quantity are listed in Table 4. The results for the simulations listed in Table 2 are plotted in Fig. 18.

Table 4. The initial rates of change of fractional change of density $\rho^{-1} \Delta \rho / \Delta t$ (where $\Delta t = 0.25$ s) and the initial values of the gradient of the fractional density $\rho^{-1} \Delta \rho / \Delta x$ (where Δx is the node spacing) for the source centers of the simulations listed in Table 2 (excepting Nos. 7 - 10). The values of $\rho^{-1} \Delta \rho / \Delta t$ correspond to the values of $\Delta \rho / \rho$ in Table 2. The gradient $\rho^{-1} \Delta \rho / \Delta x$ is that immediately upwind of the source center as in Fig. 5 and 10.

No.	$\sigma_r(m)$	$\Delta x(m)$	$\rho^{-1} \Delta \rho / \Delta t (s^{-1})$	$\rho^{-1} \Delta \rho / \Delta x (m^{-1})$
3	1	2	-1.853	+0.3631
3A	1	2	-1.023	+0.2548
11C	1	2	-0.800	+0.2252
3B	1	2	-0.539	+0.1598
11B	1	2	-0.278	+0.959
11	1	2	+0.199	-0.0816
11A	1	2	+0.312	-0.1368
6	1	1	-2.197	+0.5624
6A	1	1	-1.244	+0.3307
6B	1	1	-0.717	+0.1804
14	1	1	+0.281	-0.0694
4A	2.8	2	-1.039	+0.3120
4B	2.8	2	-0.399	+0.1541
4C	2.8	2	-0.192	+0.0804
4	2.8	2	-0.030	-0.0128
12	2.8	2	+0.032	-0.0141
5A	2.8	1	-1.221	+0.3245
5B	2.8	1	-0.448	+0.1111
5C	2.8	1	-0.215	+0.0505
5	2.8	1	-0.032	+0.0072
13	2.8	1	+0.032	-0.0076

Fig. 18. The variation of the initial rate of change of the fractional density $\rho^{-1} \Delta \rho / \Delta t$ as functions of the initial gradient of the fractional density $\rho^{-1} \Delta \rho / \Delta x$ and the geometric parameters σ_r and Δx . The values plotted are from Table 4. The dots are for $\sigma_r = 1$ m and the crosses are for $\sigma_r = 2.8$ m. The solid lines are for $\Delta x = 2$ m and the dashed line is for $\Delta x = 1$ m.

Figure 18 has several interesting features. First, a straight line could, as a rough approximation, be fitted to all 21 points. This indicates a strong correlation between $\rho^{-1}\Delta\rho/\Delta x$ and $\rho^{-1}\Delta\rho/\Delta t$ regardless of differences in simulation details. Second, the two solid lines (for $\Delta x = 2$ m) fitted to the dots (for $\sigma_r = 1$ m) from 3 to 11A and to the crosses (for $\sigma_r = 2.8$ m) from 4A to 12 are curved and slightly displaced from each other. Third, the single dashed line (for $\Delta x = 1$ m) fits both the dots (for $\sigma_r = 1$ m) from 6 to 14 and the crosses (for $\sigma_r = 2.8$ m) from 5A to 13.

In connection with Figs. 12 and 13 we found that the fractional loss of material mass can be reduced by decreasing the node spacing (Δx , Δy , Δz) and especially by setting the condition that the Gaussian source geometry parameter be greater than the node spacing ($\sigma_r > \Delta x$ and Δz , $\sigma_y > \Delta y$). We have now found another measure for control of fractional mass loss: reducing the initial density gradients in the source regions. Reduction of the quantity $(1/\rho)\Delta\rho/\Delta x$ reduces the quantity $(1/\rho)\Delta\rho/\Delta t$ which in turn reduces the quantity $\Delta M/M$ for a given time interval.

SUMMARY AND CONCLUSIONS

We have used the FEM3 model for many simulations of material dispersion from instantaneous sources and have noted changes in the total material mass during the first few seconds before any of the material could have reached an exit boundary. These failures of FEM3 to conserve material mass were considered to be acceptable if, as in most cases, the fractional mass changes were only a few percent. We initiated this study because of a few recent cases in which one-quarter to one-half of the material mass was "lost" in only a few seconds.

These failures of FEM3 to conserve mass were initially attributed to a numerical artifact associated with the linear interpolation between computational mesh nodes to determine the material mass content. The material

concentration gradients in the source region are the greatest and change rapidly at early times.

It became obvious that more must be involved when we found cases in which a large fraction of the material was "lost" in one or two seconds. The phase-change submodel was suspected to be a contributing factor because the first cases with large mass losses involved phase change. We also recalled a feature used in FEM3 to preclude sound waves: the term $\partial p / \partial t$ is not included in the mass conservation equation.

In this study we investigated the effects of varying two classes of geometric parameters: (1) the spacing in the horizontal plane between the nodes in the computational mesh (Δx and Δz), and (2) the standard deviations ($\sigma_x = \sigma_z = \sigma_r$ and σ_y) used to define the trivariate Gaussian distribution of material mass fraction about a point at zero time (the instantaneous source).

We also varied the initial density fields for the air-material mixture in the source region, with and without phase change. Very heavy mixtures were obtained with the phase-change material submodel by specifying material mass concentrations (β at the source center) that resulted in a large fraction of liquid material. Heavy mixtures were also obtained with the all-vapor material submodel by specifying lower-than-ambient initial temperatures in the source region. Lighter-than-air mixtures were added to the study using the all-vapor submodel with above-ambient source temperatures. The most useful of the simulations were those in which the air-material mixture density at the source center was unambiguously either the maximum or the minimum density in the entire field. We determined the fractional changes of the material mass ($\Delta M / M$) and the source center density ($\Delta \rho / \rho$) during the first quarter-second of the simulations. For a fixed set of geometric conditions (Δx , Δy ; σ_r , σ_y):

- o The points defining $\Delta M / M$ vs. $\Delta \rho / \rho$ form a smooth curve ranging from negative to positive values of ΔM and $\Delta \rho$ (for heavier-than-air and lighter-than-air mixtures respectively),

- o Alternating points with negative values of $\Delta M/M$ and $\Delta \rho/\rho$ from simulations with and without phase change form a single smooth curve which means that the present phase-change submodel is not in itself a cause of the non-conservation of mass.

The curves of $\Delta M/M$ vs. $\Delta \rho/\rho$ for the different combinations of geometric parameters demonstrate the following:

- o The fractional change in mass $\Delta M/M$ associated with a given fractional change in density $\Delta \rho/\rho$ was substantially reduced when the node spacing was significantly decreased (e.g., changing Δx and Δz from 2 to 1 m). This effect was much greater with $\sigma_r = 1$ m and $\sigma_y = 0.5$ m than with $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m.
- o The fractional change in mass $\Delta M/M$ for a given fractional change in density $\Delta \rho/\rho$ was substantially reduced with a change in the source geometry sigma values from less than to greater than the node spacing. (e.g. changing from $\sigma_r = 1.0$ m and $\sigma_y = 0.5$ m to $\sigma_r = 2.8$ m and $\sigma_y = 1.4$ m). This was demonstrated for $\Delta x = \Delta z = 1$ and 2 m. The node spacing along the vertical axis was the same in all cases: $0.5 \text{ m} \leq \Delta y \leq 1.18 \text{ m}$.

As noted above, the early failures of FEM3 to conserve material mass were attributed to a numerical artifact associated with the node-to-node interpolation used to determine material mass. We checked this with an isothermal, all-vapor simulation of a neutrally-buoyant material (molecular weight equal to that of air) and some similar cases which had almost-neutral buoyancy. We found a linear relation between $\Delta M/M$ and $\Delta \rho/\rho$ for values ranging from slightly less than 10^{-3} to more than 10^{-1} . There was substantial deviation from this linear relation only for values less than 10^{-4} . Therefore we were in error when we attributed the observed non-conservation of mass to numerical interpolation errors.

We conclude that the observed "losses" or "gains" in material mass are most likely a result of the omission (for a valid reason) of the $\partial p / \partial t$ term in the FEM3 mass conservation equation.

EPILOGUE

In view of the above results, Phil Gresho addressed the problem of mass conservation by FEM3 [5]. He first notes that mass cannot be conserved in models based on the much-used Boussinesq approximation. In this approximation, $\nabla \cdot \underline{u} = 0$, density is a variable only in the buoyancy term in the momentum conservation equation, and in that term density is a function of temperature and species concentration but not pressure. He then considers the anelastic approximation used to extend the capabilities of FEM3 beyond the limits of the Boussinesq approximation. In the anelastic approximation, the mass conservation equation is $\nabla \cdot (\rho \underline{u}) = 0$, density is a variable in all conservation equations, and density is a function of temperature, species concentration, and pressure through the ideal gas law. He shows that the average pressure level can be adjusted to ensure global (the sum of air and other species) mass conservation, and he proposes a change to the species conservation equation. Both modifications to FEM3 should serve to improve the material (species) conservation problem studied in this report.

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